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Learning objectives:

- Formulate axioms of QM using density operator
- Quantify entanglement of a pure quantum state
- Relate density matrices ρ to ensembles of pure states $\{p_a, |\psi_i\rangle\}$

Reduced density operator (N2.4.3, P2.3.1):

Let ρ be a density operator of a composite system $\mathcal{H}_1 \otimes \mathcal{H}_2$. Let $|i\rangle_1$ and $|i\rangle_2$ be orthonormal bases in $\mathcal{H}_1$ and $\mathcal{H}_2$, respectively.

Hilbert space 1 Hilbert space 2

We can define reduced density operators ρ_1 and ρ_2 for the two subsystems 1 and 2 as:

$$\rho_1 = \mathrm{Tr}_2\, \rho = \sum_i \left(I_1 \otimes \langle i|_2 \right) \rho \left(I_1 \otimes |i\rangle_2 \right)$$

$$\rho_2 = \mathrm{Tr}_1\, \rho = \text{accordingly.}$$

Properties of the reduced density operator:

- $\mathrm{Tr}\, \rho_1 = 1 \quad , \quad \mathrm{Tr}\, \rho_2 = 1$
- $\rho_1 \geq 0 \quad , \quad \rho_2 \geq 0$
- If $\rho = \underbrace{\sigma_1 \otimes \sigma_2}_{\text{product state}} \Rightarrow \rho_1 = \mathrm{Tr}_2\, \rho = \sigma_1$.

Examples:

① • Bell state $|\Phi^+\rangle = \frac{1}{\sqrt{2}}\left[|00\rangle + |11\rangle\right]$

$$\Rightarrow \rho = \frac{1}{2}\Big[|00\rangle + |11\rangle\Big]\Big[\langle 00| + \langle 11|\Big] =$$

$$= \begin{pmatrix} 1/2 & 0 & 0 & 1/2 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 1/2 & 0 & 0 & 1/2 \end{pmatrix}.$$

Basis

$i \in \{|00\rangle, |01\rangle, |10\rangle, |11\rangle\}.$

$$\rho_{ij} = \langle \underset{\substack{\uparrow \\ \text{row}}}{i} | \rho | \underset{\substack{\uparrow \\ \text{column}}}{j} \rangle$$

$$\text{Note } \operatorname{Tr}\rho^2 = \operatorname{Tr}\left(\begin{array}{c|cccc} & |00\rangle & |01\rangle & |10\rangle & |11\rangle \\ \hline \langle 00| & 1/2 & 0 & 0 & 1/2 \\ \langle 01| & 0 & 0 & 0 & 0 \\ \langle 10| & 0 & 0 & 0 & 0 \\ \langle 11| & 1/2 & 0 & 0 & 1/2 \end{array}\right) = 1$$

$\Rightarrow$ indeed ρ describes a pure state.

However,
$$\rho_1 = \operatorname{Tr}_2 \rho = \sum_i \langle i|_2 \rho |i\rangle_2 =$$

$$= \begin{array}{c|cc} & |0\rangle_1 & |1\rangle_1 \\ \hline \langle 0|_1 & 1/2 & 0 \\ \langle 1|_1 & 0 & 1/2 \end{array} = \frac{I}{2}$$

Thus, the purity equals

$$\mathrm{Tr}\,\rho_1^2 = \mathrm{Tr}\begin{pmatrix} 1/4 & 0 \\ 0 & 1/4 \end{pmatrix} = \frac{1}{2} < 1$$

$\Rightarrow$ ρ_1 describes mixed state (fully mixed state).

Can compute von-Neumann entanglement entropy:

eigenvalues of ρ

$$S_{VN} \equiv S = -\mathrm{Tr}\,\rho \ln \rho = -\sum_i p_i \ln p_i$$

go to eigenbasis of ρ

$\Rightarrow$ for the full system: $p_1 = 1$, $p_{2,3,4} = 0$

$\Rightarrow$ $S = 0$ (pure state carries no entropy)

$\Rightarrow$ for subsystem 1: $p_1 = p_2 = 1/2$:

$$S_1 = -2 \cdot \left(\frac{1}{2} \ln \frac{1}{2} \right) = \ln 2$$

(maximal entropy of a single qubit → fully mixed state)

② • Werner state

separable fully mixed state $\frac{I_1}{2}\otimes\frac{I_2}{2}$

$$\rho(\lambda) = \lambda\frac{I}{4} + (1-\lambda)\,|\psi^-\rangle\langle\psi^-|$$

max. entangled state

with Bell state $|\psi^-\rangle = \frac{1}{\sqrt{2}}\left[|01\rangle - |10\rangle\right]$.

Convex combination of separable state $\frac{I}{4}$ and entangled state $|\psi^-\rangle\langle\psi^-|$.

Matrix form in Z basis (computational product basis):

$$\rho(\lambda) = \begin{pmatrix} \frac{\lambda}{4} & 0 & 0 & 0 \\ 0 & \frac{1}{2}(1-\frac{\lambda}{2}) & \frac{\lambda-1}{2} & 0 \\ 0 & \frac{\lambda-1}{2} & \frac{1}{2}(1-\frac{\lambda}{2}) & 0 \\ 0 & 0 & 0 & \lambda/4 \end{pmatrix}$$

$$\frac{1}{4}\lambda + \frac{1-\lambda}{2} = \frac{1}{2} + \lambda\underbrace{\left(\frac{1}{4}-\frac{1}{2}\right)}_{=-\frac{1}{4}} = \frac{1}{2}\left(1-\frac{\lambda}{2}\right)$$

Eigenvalues:

$$p_i \in \left\{\frac{\lambda}{4}, \frac{\lambda}{4}, \frac{\lambda}{4}, 1-\frac{3}{4}\lambda\right\} \Rightarrow \lambda\in\left[0, \frac{4}{3}\right]$$

such that $\rho \geq 0$.

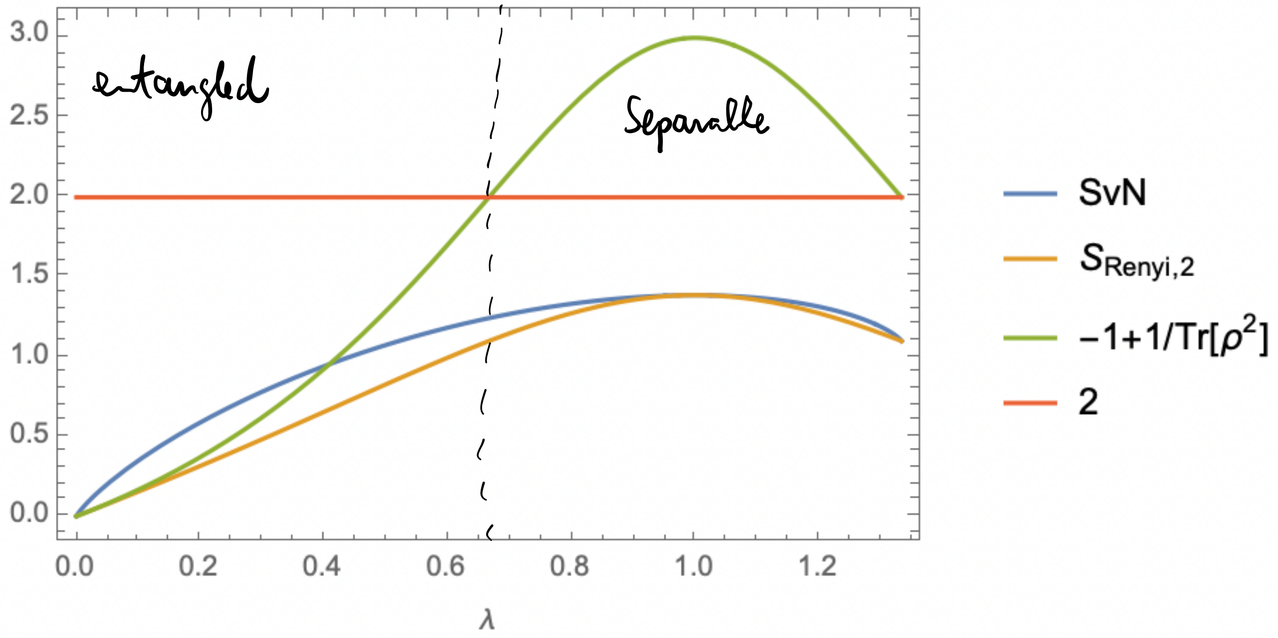
$S(\lambda=0)=0$

$\lambda = 0 : p_i \in \{1, 0, 0, 0\}$, pure state $|\psi^-\rangle\langle\psi^-|$

$\lambda = \frac{2}{3} : p_i \in \{\frac{1}{6}, \frac{1}{6}, \frac{1}{6}, \frac{1}{2}\}$, $S(\lambda = \frac{2}{3}) \approx 1.24 =$
$= \frac{1}{2}\ln 6 + \frac{1}{2}\ln 2$.

$\lambda = 1 : p_i \in \{\frac{1}{4}, \frac{1}{4}, \frac{1}{4}, \frac{1}{4}\}$: fully mixed state $\frac{I}{4}$.
$S(\lambda=1) = \ln 4 = 2\ln 2$.

$\lambda = \frac{4}{3} : p_i \in \{\frac{1}{3}, \frac{1}{3}, \frac{1}{3}, 0]$: $S(\lambda = \frac{4}{3}) = \ln 3$



Reduced density operator :

$$\rho_1 = \mathrm{Tr}_2\, \rho = \begin{array}{c|cc} & |0\rangle & |1\rangle \\ \hline \langle 0| & 1/2 & 0 \\ \langle 1| & 0 & 1/2 \end{array}$$

Always fully mixed state ⇒ can get the same density matrix in many different ways.

General question: what class of ensembles $\{p_i, |\psi_i\rangle\}$ give rise to the same density matrix ρ.

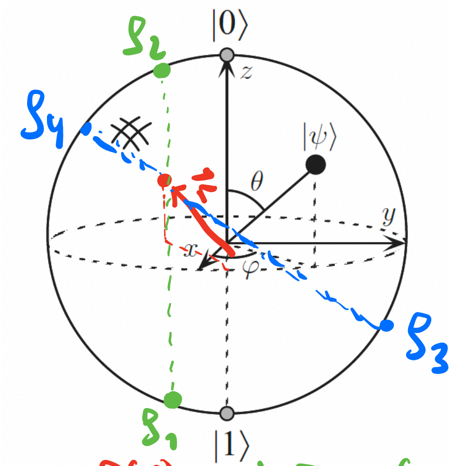
In other words: in how many ways can ρ be written as a sum of extremal states (i.e. pure states)?

First: let's look at a single qubit.

$$\rho(\vec{r}) = \frac{1}{2}(I + \vec{r}\cdot\vec{\sigma}) = \lambda\rho(\hat{m}_1) + (1-\lambda)\rho(\hat{m}_2)$$

with $\vec{r} = \lambda\hat{m}_1 + (1-\lambda)\hat{m}$.

All such chords comprise a two parameter family [i.e., the first vector $\hat{m}_1$ can be arbitrary (θ_1, ϕ_1)]



$$\rho(\vec{r}) = \lambda\rho_1 + (1-\lambda)\rho_2 = \lambda\rho_3 + (1-\lambda)\rho_4 = \dots$$

Figure 1.3. Bloch sphere representation of a qubit.

In general:

See also theorem in Hughston, Josza, Wootters, Phys. Lett. A 183 (1993).

Theorem N2.6 (unitary freedom in the ensemble for density matrices): Ensemble defined by $\mathcal{E} = \{p_i \,|\, |\psi_i\rangle\}$.

Introduce the unnormalized states $|\tilde{\psi}_i\rangle = \sqrt{p_i}\,|\psi_i\rangle$, such that

$$\rho = \sum_i p_i |\psi_i\rangle\langle\psi_i| = \sum_i |\tilde{\psi}_i\rangle\langle\tilde{\psi}_i| .$$

The sets $|\tilde{\psi}_i\rangle$ and $|\tilde{\varphi}_i\rangle$ generate the same density operator iff (if and only if)

$$|\tilde{\psi}_i\rangle = \sum_j U_{ij} |\tilde{\varphi}_j\rangle$$

where U_{ij} is a unitary matrix, and we pad whichever set of vectors $|\tilde{\psi}_i\rangle$ or $|\tilde{\varphi}_i\rangle$ is smaller with additional vectors 0 so that the two sets have the same number of elements.

$\Rightarrow$ for normalized states:

$$\rho = \sum_i p_i |\psi_i\rangle\langle\psi_i| = \sum_i q_i |\varphi_i\rangle\langle\varphi_i|$$

requires $\sqrt{p_i}\,|\psi_i\rangle = \sum_j U_{ij} \sqrt{q_j}\,|\varphi_j\rangle$

Again, pad the smaller ensemble with entries having $p_j = 0$ to make both ensembles have the same size.

Proof:

$\Rightarrow$: Suppose $|\tilde{\psi}_i\rangle = \sum_j U_{ij} |\tilde{\varphi}_j\rangle$ for unitary U_{ij}.

Then,

$$\sum_i |\tilde{\psi}_i\rangle\langle\tilde{\psi}_i| = \sum_{j,k} \underbrace{\sum_i U_{ij}\, U^*_{ik}}_{= \sum_i U_{ij} (U^\dagger)_{ki} = \delta_{jk}} |\tilde{\varphi}_j\rangle\langle\tilde{\varphi}_k| =$$

$$= \sum_j |\tilde{\varphi}_j\rangle\langle\tilde{\varphi}_j| \,. \quad \square$$

$\Leftarrow$: Conversely, suppose $\rho = \sum_i |\tilde{\psi}_i\rangle\langle\tilde{\psi}_i| = \sum_j |\tilde{\varphi}_j\rangle\langle\tilde{\varphi}_j|$.

Since $\rho^\dagger = \rho \Rightarrow$ allows for a spectral decomposition

$$\rho = \sum_k \underbrace{\lambda_k}_{>0} |\underset{\uparrow \text{orthonormal}}{k}\rangle\langle k|$$

Let's relate both $|\tilde{\psi}_i\rangle$ and $|\tilde{\varphi}_j\rangle$ to the states

$|\tilde{k}\rangle = \sqrt{\lambda_k}\, |k\rangle$.

Let $|\psi\rangle$ be any vector orthonormal to the state spanned by $\{|\tilde{k}\rangle\} \Rightarrow \langle\psi|\tilde{k}\rangle\langle\tilde{k}|\psi\rangle = 0 \;\; \forall\, \tilde{k}$.

$$\Rightarrow \langle\psi|\rho|\psi\rangle = 0 = \sum_i \langle\psi|\tilde{\psi}_i\rangle\langle\tilde{\psi}_i|\psi\rangle =$$

$$= \sum_i \underbrace{|\langle\psi|\tilde{\psi}_i\rangle|^2}_{\geq 0 \;\forall i}.$$

$\Rightarrow \langle\psi|\tilde{\psi}_i\rangle = 0 \;\; \forall\, i$ and all $|\psi\rangle \perp$ to space spanned by $\{|\tilde{k}\rangle\}$.

Thus, $|\tilde{\psi}_i\rangle$ can be expanded in terms of the $|\tilde{r}\rangle$:

$$|\tilde{\psi}_i\rangle = \sum_r c_{ir} |\tilde{r}\rangle .$$

Since

$$\rho = \sum_r |\tilde{r}\rangle\langle\tilde{r}| = \sum_i |\tilde{\psi}_i\rangle\langle\tilde{\psi}_i| =$$

$$= \sum_{r,l} \sum_i c_{ir} c^*_{il} \underbrace{|\tilde{r}\rangle\langle\tilde{l}|}$$

these operators are linearly independent as $|\tilde{r}\rangle$ are orthonormal.

$$\sum_i c_{ir} c^*_{il} = \delta_{rl} \Leftarrow$$

$$\langle\tilde{r}_1|\tilde{r}\rangle\langle\tilde{l}|\tilde{l}_1\rangle = \delta_{\tilde{r} r_1}\delta_{l l_1}$$

Assume $$|\tilde{r}\rangle\langle\tilde{l}| = \sum_{\substack{r_1 \neq \tilde{r} \\ l_1 \neq \tilde{l}}} A_{r_1 l_1} |\tilde{r}_1\rangle\langle\tilde{l}_1|$$

Now, $$\langle\tilde{r}|\tilde{r}\rangle\langle\tilde{l}|\tilde{l}\rangle = 1 = 0$$

$\Rightarrow$ cannot express this operator $|\tilde{r}\rangle\langle\tilde{l}|$ as linear combination of $|\tilde{r}_1\rangle\langle\tilde{l}_1|$ with $r_1 \neq r$, $l_1 = l$.

Since

$$\sum_i C_{ir} C^*_{il} = \delta_{rl},$$ we may append extra columns to C to obtain a unitary matrix V that fulfills

$$|\tilde{\psi}_i\rangle = \sum_r V_{ir} |\tilde{r}\rangle .$$

We have appended zero vectors to $|\tilde{r}\rangle$.

Similarly, we find unitary matrix W such that

$$|\tilde{\varphi}_j\rangle = \sum_r W_{jr} |\tilde{r}\rangle .$$

Thus, $$|\tilde{\psi}_i\rangle = \sum_j U_{ij} |\tilde{\varphi}_j\rangle$$

with unitary $U = V W^\dagger$. □

Note that a minimal ensemble $\mathcal{E} = \{ p_i \,/\, |\psi_i\rangle \}$ contains as many elements as the rank of ρ, i.e. the number of nonzero $p_i > 0$.

Summary:

n-dim. Hilbert space, spectral decomposition of ρ

$$\rho = \sum_{i=1}^{n} p_i |i\rangle\langle i|$$

$$\mathrm{rank}(\rho) = r \le n : \overbrace{p_1 \ge p_2 \ge .. p_r}^{\text{nonzero}} > \overbrace{p_{r+1} = \dots = p_n}^{\text{zero}} = 0$$

Eigenensemble of ρ : $\mathcal{E} = \{ p_i , i = 1, \dots, r \,|\, |i\rangle \}$.

- The ensemble $\{|\psi_i\}$, $i = 1, \dots, r \ge r$

$$\begin{pmatrix} |\tilde\psi_1\rangle \\ |\tilde\psi_2\rangle \\ \vdots \\ |\tilde\psi_r\rangle \end{pmatrix} = \underset{\text{unitary } r \times r \text{ matrix}}{U} \begin{pmatrix} |\tilde 1\rangle \\ \vdots \\ |\tilde r\rangle \\ |0\rangle \\ |0\rangle \\ \vdots \\ |0\rangle \end{pmatrix}$$

$$\boxed{\begin{aligned} |\tilde\psi_i\rangle &= p_i^{\frac{1}{2}} |\psi_i\rangle \\ |\tilde i\rangle &= p_i |i\rangle \end{aligned}}$$

appended $r - r$ zero states to allow U to be unitary

$$\Leftrightarrow \begin{pmatrix} |1\rangle \\ \vdots \\ |r\rangle \\ |0\rangle \\ \vdots \\ |0\rangle \end{pmatrix} = U^{-1} \begin{pmatrix} |\psi_1\rangle \\ |\psi_2\rangle \\ \vdots \\ |\psi_r\rangle \end{pmatrix}$$

This also works to go from $\{|\psi_i\rangle\}$ to $\{|\phi_i\rangle\}$.